



Thermoelectric properties of Nowotny–Juza NaZnX (X = P, As and Sb) compounds



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ABSTRACT

The electronic transport coefficients of Nowotny–Juza NaZnX (X = P, As and Sb) compounds were evaluated by using the semi-classical Boltzmann and the rigid band model. The compounds are direct band gap ($\Gamma_v - \Gamma_c$) semiconductors with energy band gaps of about 1.8, 1.47 and 0.25 eV, for NaZnX (X = P, As and Sb) respectively. A maximum value of electrical conductivity of about $5.4 \times 10^{20} (\Omega \text{ ms})^{-1}$ and $5.1 \times 10^{20} (\Omega \text{ ms})^{-1}$ is achieved at 0.2 μ (eV) for n-type of NaZnP and NaZnAs, while for NaZnSb a maximum value of about $4.1 \times 10^{20} (\Omega \text{ ms})^{-1}$ is found at -0.15μ (eV) for p-type and $4.2 \times 10^{20} (\Omega \text{ ms})^{-1}$ at 0.15μ (eV). The investigated materials exhibit the highest value of Seebeck coefficient at 300 K of about 300, 250, 510 ($\mu\text{V/K}$) for p-type and $-290, -240, -305$ ($\mu\text{V/K}$) for n-type of NaZnX (X = P, As and Sb) respectively. In the chemical potential region between $\mp 0.6, \mp 0.5, \mp 0.025 \mu$ (eV) NaZnP, NaZnAs, NaZnSb respectively exhibit a minimum value of electronic thermal conductivity. Therefore in these regions the investigated materials can give maximum efficiency.

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1. Introduction

The filled tetrahedral Nowotny–Juza NaZnX (X = P, As and Sb) compounds are promising candidates for efficient thermoelectric applications [1–8]. These material are direct band gap semiconductors which make them a good materials for photovoltaic applications [1,2]. While there exist experimental and theoretical investigation reports for the Nowotny–Juza compounds LiXY (X = Mg, Zn and Y = N, P, As), LiCdP, LiCdAs and AgMgAs, there is a dearth of information concerning NaZnX (X = P, As and Sb) compounds [9,10] especially the investigation of the thermoelectric properties of such important candidates. The thermoelectric power generators can convert heat into electricity (energy conversion) which is a good alternative solution for energy and environment problems [11]. The thermoelectric materials have gained importance in the last decade for its usefulness in energy conversion [12–14]. Recently, Charifi et al. [9] reported a theoretical study of the structural, electronic, elastic and phonon properties of NaZnX

(X = P, As and Sb) compounds using full-potential linear augmented plane wave and pseudopotential plane wave method. They used the generalized-gradient approximation (GGA), the local density approximation (LDA) and Engel–Vosko (EVGGA) formalism. They have calculated the lattice constant, bulk modulus, second-order elastic constants, the electronic band structures and the related total density of states and charge density. The authors studied three high-pressure phases and found that a transition occurs from tetragonal to a high-pressure phase. Their calculations predict that NaZnSb is a metal in all phases. Jaiganesh and Merita [10] have report first-principles tight-binding linear muffin-tin orbital method within LDA to calculate the ground-state properties, structural phase stability and pressure dependence of the band gap of NaZnX (X = P, As, Sb). They found that the three compounds crystallize in the tetragonal Cu₂Sb-type (C38) structure. They found three phases α , β and γ when they interchange the position of the atoms in the zinc-blende structure. They reported that these compounds are more stable in the Cu₂Sb-type structure under ambient conditions, whereas these compounds undergo a structural phase transition from the tetragonal Cu₂Sb-type to cubic α (or β) phase at high pressure. In the Cu₂Sb-type structure, NaZnP is found to be a direct gap semiconductor, NaZnAs shows a very small direct band gap and NaZnSb is found to be a metal. In the α and β phases, NaZnP is found to be a direct gap semiconductor, whereas NaZnAs and NaZnSb are

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found to be semi-metallic. In the γ -phase, all three compounds are found to be metallic.

From the above it is clear that the theoretical investigations were performed using LDA, GGA and EVGGA. It is well known that LDA, GGA and EVGGA underestimate the energy band gap [15] therefore this motivates us to address ourselves for a comprehensive theoretical calculation using the state-of-the-art-all-electron full potential linear augmented plane wave (FPLAPW) method, within the modified Becke–Johnson potential (mBJ) [16], which optimizes the corresponding potential for electronic band structure calculations. The modified Becke–Johnson potential allows the calculation of band gaps with accuracy similar to the very expensive GW calculations [16]. It is a local approximation to an atomic “exact-exchange” potential and a screening term. The FPLAPW method has proven to be one of the most accurate method to calculate the properties of the solid with density functional theory [17,18].

2. Details of calculation

Nowotny–Juza NaZnX (X = P, As and Sb) compounds crystallize in the tetragonal space group P4/nmm, which is the most stable phase at ambient pressure. The crystal structures of NaZnX (X = P, As and Sb) compounds are represented in Fig. 1a–c. For the electronic structure calculations the state-of-the-art full potential linear augmented plane wave (FPLAPW) method in a scalar relativistic version as embodied in the WIEN2k code [19] was used. We have employed the modified Becke–Johnson potential (mBJ) [16], which optimizes the corresponding potential for electronic band structure calculations. We have used a basis of linear APW's to solve the Kohn–Sham equations. The potential and charge density in the muffin-tin (MT) spheres were expanded in spherical harmonics with $l_{\max} = 8$ and nonspherical components up to $l_{\max} = 6$. In the interstitial region the potential and the charge density were represented by Fourier series. To achieve the self-consistency a mesh of 5000 k points in the irreducible Brillouin zone (IBZ) was used. The convergence of the total energy in the self-consistent calculations is taken with respect to the total charge of the system with a tolerance 0.0001 electron charges.

Based on the calculated electronic band structure and by the help of the semi-classical Boltzmann theory as incorporated in BoltzTraP code [20] we have calculate the thermoelectric proper-

ties using a very dense \mathbf{k} meshes of 11,560 \vec{k} points in the IBZ. The electrical conductivity $\sigma_{\alpha\beta}$, Seebeck coefficient $S_{\alpha\beta}$ and thermal conductivity (electronic part) $k_{\alpha\beta}^0$ tensors are the main transport properties. These quantities are functions of temperature (T) and chemical potential (μ) [20,21];

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{e^2}{N} \sum_{i,k} \tau_i \varepsilon \nu_{\alpha}(i, \vec{k}) \nu_{\beta}(i, \vec{k}) \delta(\varepsilon - \varepsilon_{i,k}) \quad (1)$$

where e represent charge of electron, τ is the relaxation time, α and β are the tensor indices, N is the number of \mathbf{k} -points, $\nu_{\alpha}(i, \vec{k})$ and $\nu_{\beta}(i, \vec{k})$ are the group velocities. It is important to mention that in BoltzTraP code the relaxation time τ taken as a constant [20] (typical value around 10^{-14} s). The transport coefficients can be written as a function of temperature and chemical potential [20,22] as follow:

$$\sigma_{\alpha\beta}(T, \mu) = \frac{1}{\Omega} \int \sigma_{\alpha\beta}(\varepsilon) \left[-\frac{\partial f_0(T, \varepsilon, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (2)$$

$$S_{\alpha\beta}(T, \mu) = \frac{1}{eT\Omega\sigma_{\alpha\beta}(T, \mu)} \int \sigma_{\alpha\beta}(\varepsilon) (\varepsilon - \mu) \times \left[-\frac{\partial f_0(T, \varepsilon, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (3)$$

$$k_{\alpha\beta}^0(T, \mu) = \frac{1}{e^2 T} \int \sigma_{\alpha\beta}(\varepsilon) (\varepsilon - \mu)^2 \left\{ -\frac{\partial f_0(T, \varepsilon, \mu)}{\partial \varepsilon} \right\} d\varepsilon \quad (4)$$

where Ω stands for volume of the unit cell, and f_0 is Fermi–Dirac distribution function. To gain high thermoelectric efficiency, it is important that the material possess high electrical conductivity, large Seebeck coefficient and low thermal conductivity [23].

3. Results and discussion

3.1. Salient features of the electronic band structures

The calculations of the transport properties are based on the calculated electronic band structure, therefore accurate electronic band structure gives a reliable transport properties. We will recall the main features of the electronic band structure of Nowotny–Juza NaZnX (X = P, As and Sb) compounds. As it is shown in Fig. 2 these materials possesses a direct band gap as the upper valence band and lower conduction band are situated at the center of the BZ ($\Gamma_v - \Gamma_c$). The values of these band gaps are 1.80 eV (NaZnP), 1.47 eV (NaZnAs) and 0.25 eV (NaZnSb). In general the electronic

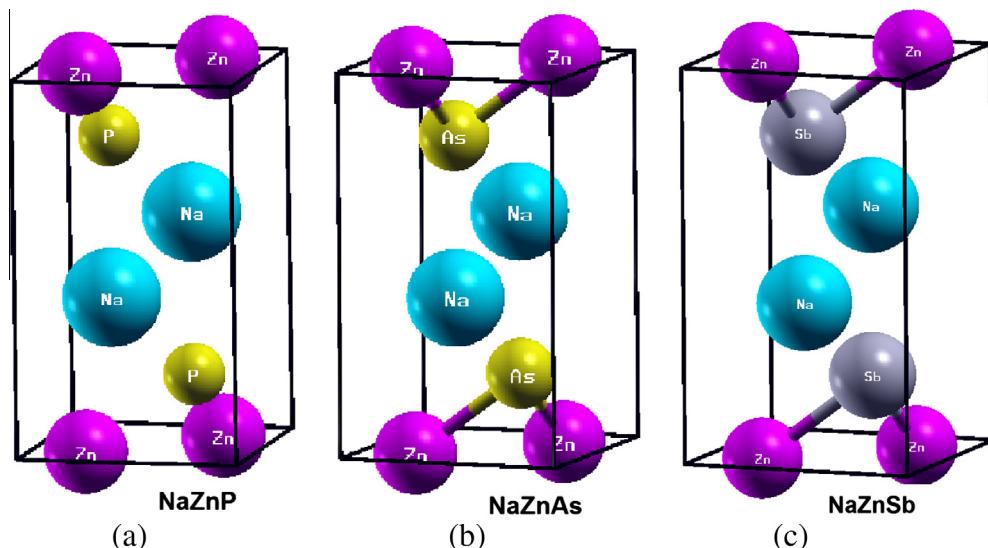


Fig. 1. Crystal structure of Nowotny–Juza NaZnX (X = P, As and Sb) compounds.

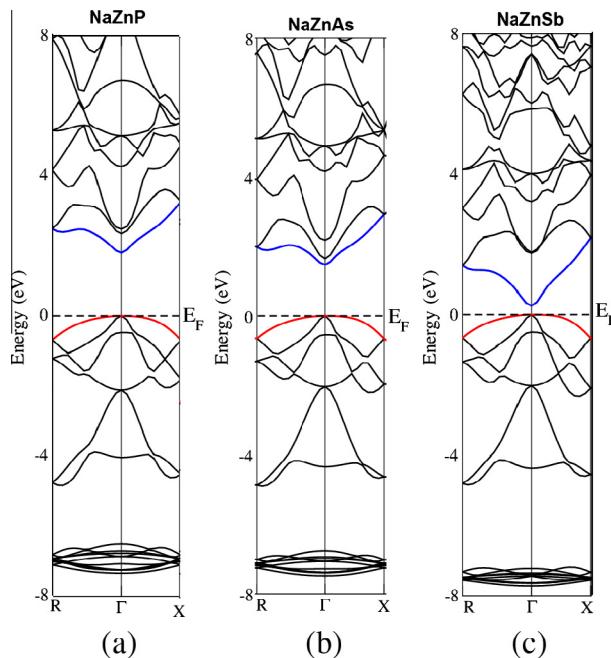


Fig. 2. The calculated electronic band structure of Nowotny–Juza NaZnX (X = P, As and Sb) compounds.

band structures of these materials are similar except that the conduction band minimum shift towards Fermi energy (E_F) when one move from P \rightarrow As \rightarrow Sb. There is a small reduction in the band gap when P is replaced by As which can be attributed to the fact that the electronegativity differences between P (2.9) and As (2.18) are very small and the atomic radii difference between P (109 pm) and As (115 pm) are also small. On the other hand the electronegativity differences between As (2.18) and Sb (2.05) and the atomic radii difference between As (115 pm) and Sb (145 pm) are significantly different, therefore there exists a large band gap reduction when As replaced by Sb.

The semiconducting character of Nowotny–Juza NaZnX (X = P, As and Sb) compounds is in accord with the fact that an direct optical gap exist in these materials extended from visible to far IR region. Our calculations differ from the previous works which report bang gaps for NaZnP of about 0.79 eV (LDA) [9], 0.64 eV [10], 0.77 eV (GGA) [9] and 1.30 eV (EVGGA) [9]. The gaps for NaZnAs are 0.44 eV (LDA) [9], 0.163 eV [10], 0.39 eV [9] and 0.79 eV (EVGGA) [9], while NaZnSb is found to be metallic. This is mainly due to the fact that LDA and GGA have simple forms that are not sufficiently flexible to accurately reproduce both the exchange–correlation energy and its charge derivative. Engel and Vosko considered this shortcoming and constructed a new functional form of GGA that is able to better reproduce the exchange potential at the expense of less agreement in the exchange energy. But it still underestimates the band gap. Therefore, in our calculations we introduce the mBJ which allows the calculation of band gaps with accuracy similar to the very expensive GW calculations [16]. It is a local approximation to an atomic “exact-exchange” potential and a screening term.

3.2. Effective mass

The effective masses and effective masses ratio of Nowotny–Juza NaZnX (X = P, As and Sb) compounds were obtained from the curvature of the upper valence bands and the lower conduction band in the vicinity of Γ point (see Fig. 2). The effective masses can be obtained through a simple parabolic fitting using the definition

of effective mass as a second derivative of energy band with respect to the wave vector, k :

$$\frac{1}{m^*} = \frac{\partial^2 E(k)}{\hbar^2 \partial k^2} \quad (5)$$

We can calculate the curvature of the upper valence bands using the following approach: if the spin–orbit interaction were neglected, the top of the valence band would have a parabolic behavior in the vicinity of the point Γ . The materials under investigation satisfy the parabolic condition of the upper valence bands at Γ point. The calculated electron effective mass ratio (m_e^*/m_e), heavy holes (m_{hh}^*/m_e) and light holes (m_{lh}^*/m_e) effective masses ratio were presented in Table 1. We can say in some approximate way that an electron in a solid moves as if it were a free electron but with an effective mass m^* rather than a free electron mass. The larger the band curvature, the smaller the effective mass.

It is quite clear from Fig. 2a–c that the valence bands are less dispersive in all the high symmetry directions. This would imply larger effective mass for the carriers belonging to these bands and hence a high Seebeck coefficient. However, presence of carriers with large mobility is required for obtaining a higher electrical conductivity (σ). The thermoelectric power factor ($S^2\sigma/\tau$) is indirectly related to the effective mass through $\sigma = ne(\mu_e + \mu_h)$ where $\mu_e = e\tau_e/m_e^*$ and $\mu_h = e\tau_h/m_h^*$ [24]. Therefore the thermoelectric power factor can be improved, if the effective mass is increased, because the gain in Seebeck coefficient is larger than the decrease in the mobility [25]. The main factors to determine the transport properties are the effective charge–carrier’s mass, the Seebeck coefficient and electrical conductivity of materials. The electron mobility characterizes how quickly an electron can move through a metal or semiconductor.

3.3. Thermoelectric properties

To achieve the highest electrical conductivity, material should have highest mobility carriers. This can be achieved by increasing the material’s temperature which leads to an increase in the mobility of the charge carriers resulting in increase in the electrical conductivity $\sigma = ne\mu$ where $\mu_e = e\tau_e/m_e^*$ and $\mu_h = e\tau_h/m_h^*$. Following these formulas, materials with small effective masses possess high mobility carriers. The electrical conductivity is directly related to the charge carriers concentration. The total carrier concentration is defined as the difference between the hole and the electron concentration. The electron and holes carrier concentration are define as [26]:

$$p = \frac{2}{\Omega} \int_{BZ} \int_{VB} [1 - f_0(T, \varepsilon, \mu)] d\varepsilon \quad (6)$$

$$n = \frac{2}{\Omega} \int_{BZ} \int_{CB} f_0(T, \varepsilon, \mu) d\varepsilon \quad (7)$$

In the above equation, the integral is performed over the Brillouin Zone (BZ) as well as over conduction band (CB) for electrons (n) or valence band (VB) for holes (p).

Table 1

Calculated the electron effective mass ratio (m_e^*/m_e), effective mass of the heavy holes (m_{hh}^*/m_e) and light holes (m_{lh}^*/m_e), around Γ point the center of the BZ for Nowotny–Juza NaZnX (X = P, As and Sb) compounds.

Compound	m_e^*/m_e	m_{hh}^*/m_e	m_{lh}^*/m_e
NaZnP	0.006108	0.10067	0.00403
NaZnAs	0.00566	0.11668	0.00348
NaZnSb	0.00473	0.09588	0.00252

The charge carriers concentration of NaZnX ($X = \text{P, As and Sb}$) compounds as a function of temperature is illustrated in Fig. 3a. It is clear that the charge carrier concentration increases with increasing the temperature. NaZnP exhibit the highest carrier concentration along the temperature scale, while NaZnAs and NaZnSb show the same trends up to 300 K. Above this temperature NaZnAs shows higher carrier concentration than that obtained from NaZnSb .

The electrical conductivity as a function of chemical potential at two constant temperatures (300 and 600) K were obtained for NaZnX ($X = \text{P, As and Sb}$) compounds as presented in Fig. 3b–d. Following these figures one can see that the critical points of the chemical potential for the electrical conductivity in p-type and n-type region of NaZnP and NaZnAs compounds are $\pm 0.2 \mu \text{eV}$, while for NaZnAs the critical points are $\pm 0.15 \mu \text{eV}$. We should emphasize that NaZnP and NaZnAs compounds show the highest electrical conductivity of about $5.4 \times 10^{20} (\Omega \text{ ms})^{-1}$ and $5.1 \times 10^{20} (\Omega \text{ ms})^{-1}$ at $0.2 \mu \text{eV}$ n-type. For NaZnSb the highest value of electrical conductivity of is about $4.1 \times 10^{20} (\Omega \text{ ms})^{-1}$ at $-0.15 \mu \text{eV}$ p-type and $4.2 \times 10^{20} (\Omega \text{ ms})^{-1}$ $0.15 \mu \text{eV}$ n-type. It is clear that both of NaZnP and NaZnAs exhibit the same trends of the variation of the chemical potential with temperature, whereas NaZnSb shows a different behavior that is attributed to the size of the energy gaps.

The calculated Seebeck coefficient (S) of the investigated compounds as a function of chemical potential at 300 and 600 K are illustrated in Fig. 3e–g. The positive Seebeck coefficient is related to p-type charge carrier, and the negative Seebeck coefficient represent the n-type charge carrier. At the vicinity of Fermi level the Seebeck coefficient exhibit two pronounced peaks for n-/p-types. The investigated materials give the highest S at 300 K. These values are 300, 250 and 510 ($\mu\text{V/K}$) for p-type of NaZnP , NaZnAs , and NaZnSb , respectively. While for n-type NaZnP , NaZnAs , and NaZnSb , the values are -290 , -240 , -305 ($\mu\text{V/K}$), respectively. It is clear that NaZnSb exhibits the highest S in p-/n-type regions, that is due to the fact that NaZnSb possess very small gap of about 0.25 eV. We should highlight that the critical points of Seebeck coefficient for p-type and n-type of NaZnP and NaZnAs are $\pm 0.2 \mu \text{eV}$, whereas for NaZnSb these points are $\pm 0.15 \mu \text{eV}$. The critical points represent the range where the materials exhibit good thermoelectric properties, and beyond these points S is vanishes.

Usually the thermal conductivity ($k = k_e + k_l$) consist of two parts, k_e is the electronic part k_e (electrons and holes transporting heat) and k_l is phonon part (phonons traveling through the lattice). We should emphasize that the BoltzTraP code calculates only the electronic part k_e . The good and efficient thermoelectric devices were made of materials possess low thermal conductivity. We have

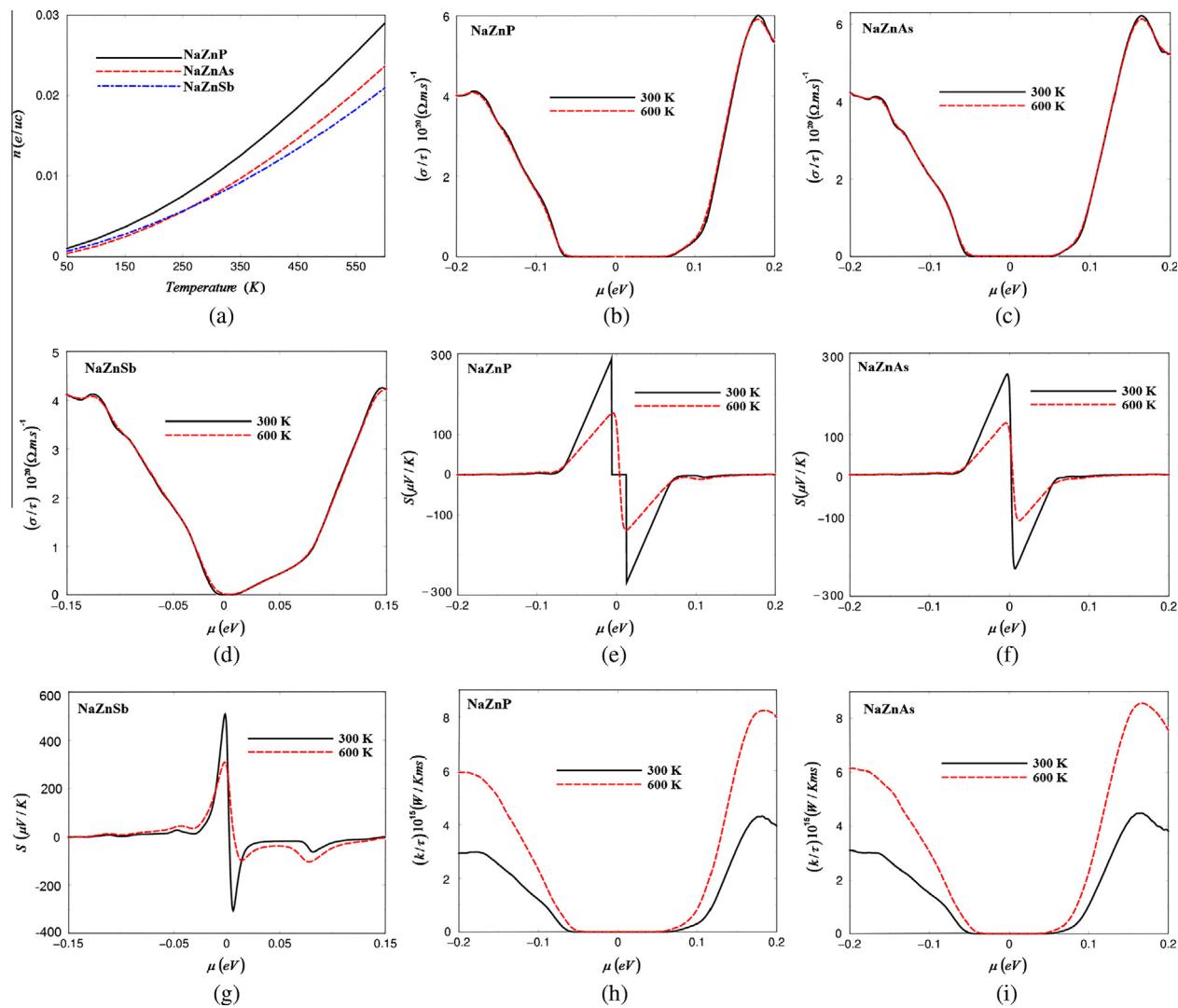


Fig. 3. The calculated transport properties as a function of chemical potential at three constant temperatures 300 and 600 K for Nowotny–Juza NaZnX ($X = \text{P, As and Sb}$) compounds: (a) carriers concentration; (b)–(d) electrical conductivity; (e)–(g) Seebeck coefficient; (h)–(j) electronic thermal conductivity; (k)–(m) power factor.

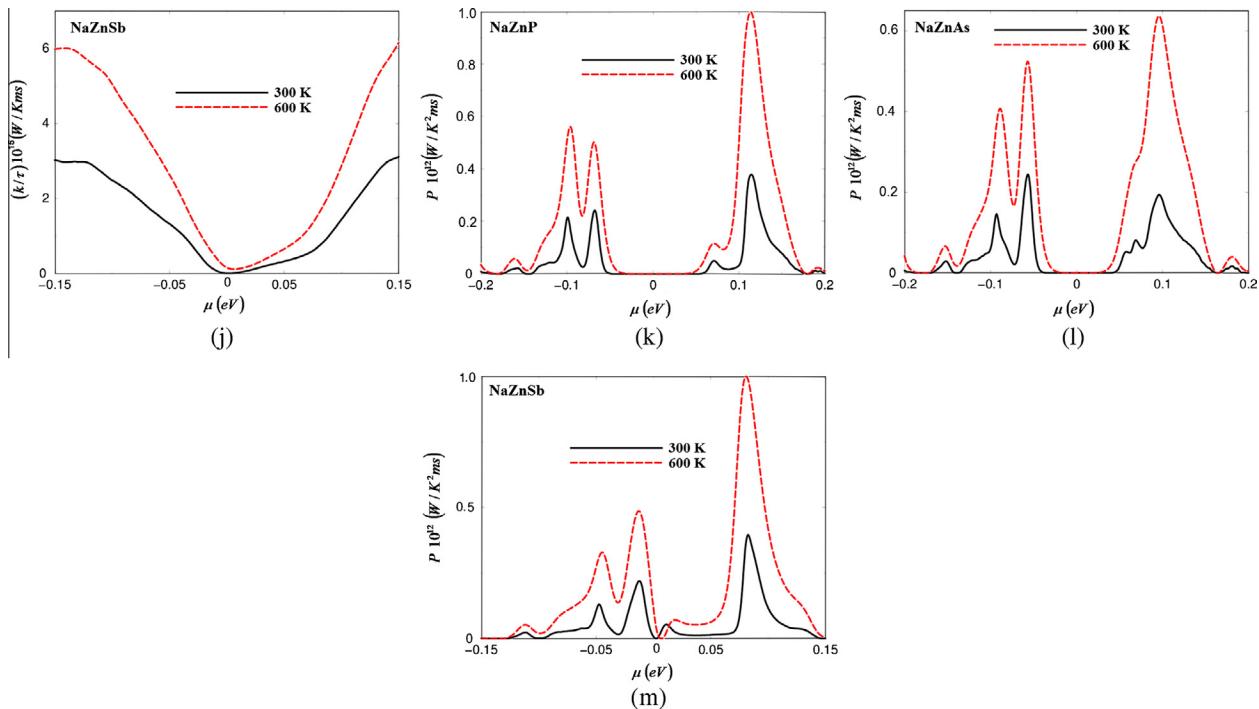


Fig. 3 (continued)

Table 2

The maximum values of the electronic thermal conductivity at $\pm 0.2 \mu$ (eV) for NaZnP and NaZnAs, and at $\pm 0.15 \mu$ (eV) for NaZnSb.

Temp. (K)	NaZnP		NaZnAs		NaZnSb	
	p-type ($\times 10^{16}$) (W/K ms)	n-type ($\times 10^{16}$) (W/K ms)	p-type ($\times 10^{16}$) (W/K ms)	n-type ($\times 10^{16}$) (W/K ms)	p-type ($\times 10^{16}$) (W/K ms)	n-type ($\times 10^{16}$) (W/K ms)
300	0.30	0.40	0.31	0.39	0.30	0.31
600	0.60	0.80	0.62	0.77	0.60	0.61

calculated the electronic thermal conductivity for Nowotny–Juza NaZnX (X = P, As and Sb) compounds at three different temperatures vs. the chemical potential as shown in Fig. 3h–j. At the chemical potential ranges between $\pm 0.6 \mu$ (eV), $\pm 0.5 \mu$ (eV) and $\pm 0.025 \mu$ (eV), NaZnP, NaZnAs and NaZnSb, respectively exhibit a minimum value of thermal conductivity, which is present in the regions where the investigated materials can give its maximum efficiency. Table 2 presents the electronic thermal conductivity for p-type and n-type of the investigated materials at 300 and 600 K, which shows that the p-/n-types of investigated materials exhibit almost the same values of electronic thermal conductivity.

The power factor (P) is directly proportional to the Seebeck coefficient square times electrical conductivity ($P = S^2 \sigma$). It is very important quantity for calculating the transport properties of the materials because it comes as a numerator in the figure of merit relation ($ZT = S^2 \sigma T / \kappa_e$). The power factor of Nowotny–Juza NaZnX (X = P, As and Sb) compounds were calculated at 300 and 600 K as a function of chemical potential between $\pm 0.2 \mu$ (eV) for NaZnP and NaZnAs, whereas it is between $\pm 0.15 \mu$ (eV) for NaZnSb as illustrated in Fig. 3k–m. At the vicinity of Fermi level the power factor exhibit the minimum values that is attributed to fact that σ shows the minimum values in the vicinity of Fermi level and beyond that the power factor increases rapidly to form two pronounced peaks for p-/n-type of the investigated materials. These peaks are located at $\pm 0.05 \mu$ (eV) for NaZnP and NaZnAs, while for NaZnSb the peaks are located at $\pm 0.05 \mu$ (eV) for p-type and around $\pm 0.075 \mu$ (eV) for n-type. For all compounds the highest

Table 3

The peaks position of the power factor in (eV).

Temp. (K)	NaZnP		NaZnAs		NaZnSb	
	p-type	n-type	p-type	n-type	p-type	n-type
300	0.20	0.30	0.25	0.20	0.20	0.35
600	0.60	1.00	0.50	0.65	0.50	1.00

power factor occurs at 600 K, thereafter it decreases with decreasing the temperature. The values of these peaks are listed in Table 3.

4. Conclusions

Based on the state-of-the-art full potential linear augmented plane wave method within the modified Becke–Johnson potential (mBJ), we have performed calculations of the thermoelectric properties for the Nowotny–Juza NaZnX (X = P, As and Sb) compounds using the semi-classical Boltzmann theory as incorporated in BoltzTraP code. Calculations show that these materials possesses a direct band gap as the upper valence band and lower conduction band are situated at the center of the BZ ($\Gamma_v - \Gamma_c$). The values of these band gaps are 1.80 eV (NaZnP), 1.47 eV (NaZnAs) and 0.25 eV (NaZnSb). We should emphasize that previous calculations using LDA, GGA and EVGGA found that NaZnSb is metallic which is attributed to the well-known underestimations of these approaches.

The maximum value of electrical conductivity of about $5.4 \times 10^{20} (\Omega \text{ ms})^{-1}$ and $5.1 \times 10^{20} (\Omega \text{ ms})^{-1}$ is achieved at 0.2μ (eV) for n-type of NaZnP and NaZnAs, while for NaZnSb achieved maximum value of about $4.1 \times 10^{20} (\Omega \text{ ms})^{-1}$ at -0.15μ (eV) for p-type and $4.2 \times 10^{20} (\Omega \text{ ms})^{-1}$ at 0.15μ (eV). The investigated materials exhibit the highest value of Seebeck coefficient at 300 K. In the chemical potential region between ± 0.6 , ± 0.5 , $\pm 0.25 \mu$ (eV) NaZnP, NaZnAs, NaZnSb respectively they exhibit minimum value of electronic thermal conductivity. Therefore in these regions the investigated materials can give its maximum efficiency.

Acknowledgments

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